

chain nodes: 7 8 9 10

ring nodes :

1 2 3 4 5 6 13 14 15 16 17

chain bonds :

6-7 7-8 8-9 8-10 9-13

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 13-14 13-17 14-15 15-16 16-17

exact/norm bonds :

1-2 1-6 2-3 3-4 4-5 5-6 6-7 8-9 8-10 9-13 13-14 13-17 14-15 15-16 16-17

exact bonds :

7-8

Match level :

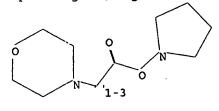
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS

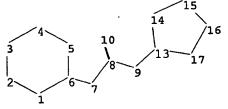
13:Atom 14:Atom 15:Atom 16:Atom 17:Atom

L1 STRUCTURE UPLOADED

=>

Uploading C:\Program Files\Stnexp\Queries\10765267pt2.str





chain nodes :
7 8 9 10
ring nodes :

1 2 3 4 5 6 13 14 15 16 17

chain bonds :

6-7 7-8 8-9 8-10 9-13

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 13-14 13-17 14-15 15-16 16-17

exact/norm bonds :

1-2 1-6 2-3 3-4 4-5 5-6 6-7 8-9 8-10 9-13 13-14 13-17 14-15 15-16 16-17

exact bonds :

7-8

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom

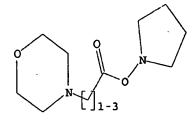
L2 STRUCTURE UPLOADED

=> d 12

L2 HAS NO ANSWERS

L2

STR



Structure attributes must be viewed using STN Express query preparation.

=> s 12

SAMPLE SEARCH INITIATED 15:00:11 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 8 TO ITERATE

100.0% PROCESSED

8 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

COMPLETE BATCH

329

0

PROJECTED ITERATIONS: 8 TO 0 TO

PROJECTED ANSWERS:

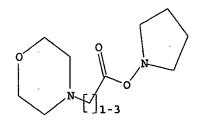
0 SEA SSS SAM L2

=> d l1

L3

L1 HAS NO ANSWERS

Ll STR



Structure attributes must be viewed using STN Express query preparation.

SAMPLE SEARCH INITIATED 15:00:34 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 8 TO ITERATE

100.0% PROCESSED

8 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS:

8 TO 329

PROJECTED ANSWERS:

O TO

L4

0 SEA SSS SAM L1

=> s l1 full

FULL SEARCH INITIATED 15:00:40 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 172 TO ITERATE

100.0% PROCESSED

172 ITERATIONS

6 ANSWERS

SEARCH TIME: 00.00.01

6 SEA SSS FUL L1

=> fil hcaplus

COST IN U.S. DOLLARS

TOTAL SINCE FILE

ENTRY

SESSION

FULL ESTIMATED COST

163.05 163.26

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FILE COVERS 1907 - 8 Sep 2005 VOL 143 ISS 11 FILE LAST UPDATED: 7 Sep 2005 (20050907/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> .s 15

L6 4 L5

=> d ed abs ibib hitstr 1-4

```
ANSWER 1 OF 4 HCAPLUS COPYRIGHT 2005 ACS on STN
L6
     Entered STN: 08 Oct 2004
ED
     Provided is a method for characterizing a mol. by mass spectrometry, which
AB
    mol. comprises one or more free amino groups, which method comprises: (a)
     reacting one or more free amino groups in the mol. with a mass tag reagent
     comprising a reactive functionality capable of reacting with an amino
     group, and a tertiary amino group linked to the reactive functionality;
     and (b) characterizing the mol. by mass spectrometry.
                         2004:824132 HCAPLUS
ACCESSION NUMBER:
DOCUMENT NUMBER:
                         141:310231
                         Mass labels
TITLE:
                         Hamon, Christian; Kuhn, Karsten; Thompson, Andrew;
INVENTOR(S):
                         Reuschling, Dieter; Schaefer, Juergen
PATENT ASSIGNEE(S):
                        Xzillion G.m.b.H. & Co. K.-G., Germany; Proteome
                         Sciences PLC
SOURCE:
                         PCT Int. Appl., 63 pp.
                         CODEN: PIXXD2
DOCUMENT TYPE:
                         Patent
                         English
LANGUAGE:
FAMILY ACC. NUM. COUNT:
PATENT INFORMATION:
     PATENT NO.
                        KIND DATE
                                            APPLICATION NO.
                                                                   DATE
                         ---
     WO 2004086050
                                20041007
                                            WO 2004-GB1167
                                                                   20040318
                         A2
                                20041229
     WO 2004086050
                         A3
         W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
             LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
             NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
             TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ,
             BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE,
             ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI,
             SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN,
             TD, TG
PRIORITY APPLN. INFO.:
                                            GB 2003-6756
                                                                A 20030324
     741683-76-1P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (mass labels)
RN
     741683-76-1 HCAPLUS
     2,5-Pyrrolidinedione, 1-[(4-morpholinylacetyl)oxy]- (9CI)
                                                                (CA INDEX NAME)
CN
```

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Ngrazier 10765267
    ANSWER 2 OF 4 HCAPLUS COPYRIGHT 2005 ACS on STN
L6
    Entered STN: 20 Aug 2004
ED
    This invention pertains to methods, mixts., kits and/or compns. for the
AB
     determination of analytes by mass anal. using unique labeling reagents or sets of
     unique labeling reagents. The labeling reagents can be isomeric or
     isobaric and can be used to produce mixts. suitable for multiplex anal. of
     the labeled analytes.
ACCESSION NUMBER:
                         2004:681717 HCAPLUS
DOCUMENT NUMBER:
                         141:202794
TITLE:
                         Methods, mixtures, kits and compositions pertaining to
                         analyte determination
                         Pappin, Darryl J. C.; Bartlet-Jones, Michael
INVENTOR(S):
PATENT ASSIGNEE(S):
                         Applera Corporation, USA
                         PCT Int. Appl., 105 pp.
SOURCE:
                         CODEN: PIXXD2
                         Patent
DOCUMENT TYPE:
                         English
LANGUAGE:
FAMILY ACC. NUM. COUNT:
PATENT INFORMATION:
     PATENT NO.
                         KIND
                                DATE
```

DATE APPLICATION NO. -----_ _ _ _ WO 2004-US2077 20040127 A2 20040819 WO 2004070352 W: AE, AE, AG, AL, AL, AM, AM, AM, AT, AT, AU, AZ, AZ, BA, BB, BG, BG, BR, BR, BW, BY, BY, BZ, BZ, CA, CH, CN, CN, CO, CO, CR, CR, CU, CU, CZ, CZ, DE, DE, DK, DK, DM, DZ, EC, EC, EE, EE, EG, ES, ES, FI, FI, GB, GD, GE, GE, GH, GM, HR, HR, HU, HU, ID, IL, IN, IS, JP, JP, KE, KE, KG, KG, KP, KP, KP, KR, KZ, KZ, KZ, LC, LK, LR, LS, LS, LT, LU, LV, MA, MD, MD, MG, MK, MN, MW, MX, MX, MZ, MZ, NA, NI RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ; UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG 20040819 CA 2004-2488584 20040127 CA 2488584 AA 20040127 20041104 US 2004-765264 US 2004219685 **A1** US 2004-765267~ 20040127 US 2004220412 **A1** 20041104 20040127 US 2004219686 **A1** 20041104 US 2004-765458 US 2003-443612P Р 20030130 PRIORITY APPLN. INFO.: 20040127 WO 2004-US2077

741683-76-1P 741683-77-2P 741683-78-3P IT

RL: SPN (Synthetic preparation); PREP (Preparation)

(methods, mixts., kits and compns. pertaining to analyte determination) 741683-76-1 HCAPLUS

2,5-Pyrrolidinedione, 1-[(4-morpholinylacetyl)oxy]- (9CI) (CA INDEX NAME) CN

RN 741683-77-2 HCAPLUS

2,5-Pyrrolidinedione, 1-[(4-morpholinylacetyl-1-13C)oxy]- (9CI) (CA INDEX

RN 741683-78-3 HCAPLUS CN 2,5-Pyrrolidinedione, 1-[(4-morpholinylacetyl-2-13C)oxy]- (9CI) (CA INDEX NAME)

ANSWER 3 OF 4 HCAPLUS COPYRIGHT 2005 ACS on STN Entered STN: 30 May 1997 L6

ED

AB _ The title polymers having a single reactive mojety at one end of the polymer chain have the following structure R-Z-X-Y (R = N-acryloylmorpholine residue with d.p. 6-280, which yields number-average mol. weight 1000-40,000; Z-X-Y = polymer capping moiety; X = saturated residue of linear or branched aliphatic series CrH2r, r' = 1-12; Y = reactive moiety, such as -OH, -CO2H, or -NH2; Z = moiety that readily reacts to cap a polymer free radical, e.g., S). The monofunctional polymer is a suitable alternative to monofunctional PEG for modification of substances having biol. and biotech. applications.

1997:341994 HCAPLUS ACCESSION NUMBER:

127:34643 DOCUMENT NUMBER:

Polymers of N-acryloylmorpholine derivative activated TITLE:

at one end and conjugates with bioactive materials and

surfaces

INVENTOR(S): Veronese, Francesco M.; Schiavon, Oddone; Caliceti,

Paolo; Sartore, Luciana; Ranucci, Elisabetta; Ferruti,

PATENT ASSIGNEE(S): Consiglio Nazionale Delle Ricerche, Italy

SOURCE:

U.S., 9 pp.

DOCUMENT TYPE:

CODEN: USXXAM Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5629384	A	19970513	US 1994-243869	19940517
US 5631322	Α	19970520	US 1995-475177	19950607
PRIORITY APPLN. INFO.:			US 1994-243869 F	3 19940517

IT 190727-27-6P

> RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); IMF (Industrial manufacture); PRP (Properties); BIOL (Biological study); PREP (Preparation)

(polymers of N-acryloylmorpholine derivative activated at one end and conjugates with bioactive materials and surfaces)

RN 190727-27-6 HCAPLUS

Morpholine, 4-[4-[(2,5-dioxo-1-pyrrolidinyl)oxy]-1,4-dioxo-2-butenyl]-, CN homopolymer (9CI) (CA INDEX NAME)

CM

CRN 190727-26-5 CMF C12 H14 N2 O6

ANSWER 4 OF 4 HCAPLUS COPYRIGHT 2005 ACS on STN L6

Entered STN: 12 May 1984

ED GI

Spectinomycylamines I [R = alkyl, optionally substituted CH2Ph, AΒ cyclohexyl, oxoalkyl, hydroxyalkyl, optionally substituted benzoylalkyl, acyl, aminoalkyl, amino(hydroxy)alkyl, amino(oxo)alkyl, carbamoylphenyl; R1 = H, Me] were prepared and showed bactericidal activity. Thus 6,8-bis(benzyloxycarbonyl) spectinomycin was treated with Me2CHNH2 and NaB(CN)H3, and the product was subjected to hydrogenolysis to give I (R = CHMe2, R1 = H), which had a ED50 against Escherichia coli ATCC 11775 of 9 mg/kg s.c. in mice.

ACCESSION NUMBER: 1980:639849 HCAPLUS

93:239849 DOCUMENT NUMBER:

Spectinomycylamines and pharmaceutical compositions TITLE:

containing them

INVENTOR (S):

Woitun, Eberhard; Maier, Roland; Reuter, Wolfgang; Wetzel, Bernd; Goeth, Hanns; Lechner, Uwe; Werner, Uwe

Thomae, Dr. Karl, G.m.b.H., Fed. Rep. Ger. PATENT ASSIGNEE(S):

Ger. Offen., 102 pp. SOURCE:

CODEN: GWXXBX

DOCUMENT TYPE: Patent

German LANGUAGE:

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE			
DE 2851953	A1	19800619	DE 1978-2851953	19781201			
PRIORITY APPLN. INFO.:			DE 1978-2851953 A	19781201			
IT 75727-76-3							
RL: RCT (Reactant); RACT (Reactant or reagent)							
(N-acylation of bis(benzyloxycarbonyl)spectinomycylamine by)							

75727-76-3 HCAPLUS RN

2,5-Pyrrolidinedione, 1-[3-(4-morpholinyl)-1-oxopropoxy]- (9CI) (CA INDEX CN NAME)

=> log y		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	24.66	187.92
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-2.92	-2.92

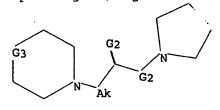
STN INTERNATIONAL LOGOFF AT 15:01:51 ON 08 SEP 2005

=> screen 2039

SCREEN CREATED L1

=> .

Uploading C:\Program Files\Stnexp\Queries\expand10765267.str



10

chain nodes : 7 8 9 10 ring nodes : 1 2 3 4 5 6 11 12 13 14 15 chain bonds : 6-7 7-8 8-9 8-10 9-11

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 11-12 11-15 12-13 13-14 14-15

exact/norm bonds :

1-2 1-6 2-3 3-4 4-5 5-6 6-7 7-8 8-9 8-10 9-11 11-12 11-15 12-13 13-14

14-15

isolated ring systems : containing 1 : 11 :

G1:C,N

G2:0,S

G3:C,O,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom

STRUCTURE UPLOADED L2

=> que L2 AND L1

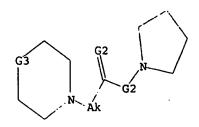
L3 QUE L2 AND L1

=> d 13

L3 HAS NO ANSWERS

SCR 2039 Ll

STR L2



G1 C,N

G2 0, S

·G3 C, O, N

Structure attributes must be viewed using STN Express query preparation. L3 QUE L2 AND L1

=> s 13

SAMPLE SEARCH INITIATED 15:50:49 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 0 TO ITERATE

100.0% PROCESSED

0 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS:

0 TO 0

PROJECTED ANSWERS:

0 TO 0

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O SEA SSS SAM L2 AND L1

=> s 13 full

FULL SEARCH INITIATED 15:50:54 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 29 TO ITERATE

9 SEA SSS FUL L2 AND L1

100.0% PROCESSED

29 ITERATIONS

9 ANSWERS

SEARCH TIME: 00.00.01

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=> fil hcaplus
COST IN U.S. DOLLARS

SINCE FILE TOTAL

164.77

ENTRY SESSION

164.98

FULL ESTIMATED COST

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 15

L6 7 L5

=> d ed abs ibib hitstr 1-7

L6 ANSWER 1 OF 7 HCAPLUS COPYRIGHT 2005 ACS on STN

ED Entered STN: 08 Jul 2005

GI

EFO 1/30/03

DATE

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Isotopically enriched N-substituted piperazines (I) or salts thereof, ΔR comprising one or more heavy atom isotopes (Y = straight chain or branched C1-6 alkyl or C1-6 alkyl ether group wherein the carbon atoms of the alkyl group or alkyl ether group each independently comprise linked hydrogen, deuterium or fluorine atoms; Z = independently H, F, Cl, Br, iodine, an amino acid side chain, a straight chain or branched C1-6 alkyl group that may optionally contain a substituted or unsubstituted aryl group wherein the carbon atoms of the alkyl and aryl groups each independently comprise linked H or F atoms, a straight chain or branched C1-6 alkyl ether group that may optionally contain a substituted or unsubstituted aryl group (wherein the carbon atoms of the alkyl and aryl groups each independently comprise linked hydrogen or fluorine atoms), or a straight chain or branched C1-6 alkoxy group that may optionally contain a substituted or unsubstituted aryl group; wherein the carbon atoms of the alkyl and aryl groups each independently comprise linked hydrogen or fluorine atoms; wherein the N-methylpiperazine is isotopically enriched with either of 13C and/or 15N) are prepared N-substituted piperazines can be used as intermediates in the synthesis of N-substituted piperazine acetic acids which in turn can be used as intermediates in the synthesis of active esters of N-substituted piperazine acetic acid. The active esters of N-substituted piperazine acetic acid can be used as labeling reagents to prepare a set of isobaric labeling reagents. The set of isobaric labeling reagents can be used to label analytes such as peptides, proteins, amino acids, oligonucleotides, DNA, RNA, lipids, carbohydrates, steroids, small mols. and the like (no data). Thus, to a stirring solution of 1.18 g (11.83 mmol) N-methylpiperazine in 15 mL toluene at room temperature was added 1 g (5.91 mmol) of Et bromoacetate-1,2-13C dropwise, over a period of 15 min. The reaction mixture was then heated in an oil bath at 90° for 4 h, cooled to room temperature, filtered to remove the off-white solid to give, after workup on the combined filtrate and washings, 1.10 g (quant.) of 4-methylpiperazine-1-acetic acid Et ester-1,2-13C (II) as an off-white oil. II (1.1 g) was refluxed in water for 24 h to give 780 mg 4-methylpiperazine-1-acetic acid-1,2-13C.

ACCESSION NUMBER: 2005:592130 HCAPLUS

DOCUMENT NUMBER: 143:115574

TITLE: Preparation of isotopically enriched N-substituted

piperazines

INVENTOR(S): Pappin, Darryl J. C.; Pillai, Sasi; Coull, James M.

PATENT ASSIGNEE(S): Applera Corp., USA

SOURCE: U.S. Pat. Appl. Publ. 29 pp. CODEN: USXXCO

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 6

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO.

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                               20050707
                                           US 2004-751388
                                                                  20040105
                         A1
    US 2005148773
                        A1
                               20050728
                                           WO 2005-US223
                                                                  20050105
    WO 2005068446
        W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
            CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
            GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
            LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
            NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
            TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
        RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
            AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
            EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT,
            RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML,
            MR, NE, SN, TD, TG
PRIORITY APPLN. INFO.:
                                           US 2004-751353
                                                               A 20040105
                                           US 2004-751354 V
                                                               A 20040105
                                           US 2004-751387
                                                               A 20040105
                                           US 2004-751388
                                           US 2004-822639
                                                                  20040412
                                           US 2004-852730
                                                               A 20040524
    856188-20-0P
    RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST
     (Analytical study); PREP (Preparation); USES (Uses)
        (preparation of isotopically enriched N-substituted piperazines as isobaric
       labeling reagents)
     856188-20-0 HCAPLUS
RN
    2.5-Pyrrolidinedione, 1-[[(4-methyl-1-piperazinyl-1-15N)acetyl-2-13C-
CN
     180]oxy]-, dihydrochloride (9CI) (CA INDEX NAME)
```

•2 HCl

●2 HCl

IT 856187-87-6P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of isotopically enriched N-substituted piperazines as isobaric labeling reagents)

RN 856187-87-6 HCAPLUS

CN 2,5-Pyrrolidinedione, 1-[[(4-methyl-1-piperazinyl)acetyl-180]oxy]- (9CI)
(CA INDEX NAME)

ANSWER 2 OF 7 HCAPLUS COPYRIGHT 2005 ACS on STN L6

Entered STN: 08 Jul 2005 ED

GI

In some embodiments, this invention pertains to active esters of AB N-substituted piperazine acetic acid I (R = leaving group; X = 0, S; Y = C1-C6 alkyl, C1-C6 alkyl ether; Z = H, 2H, F, Cl, Br, iodide, amino acid side chain, C1-C6 alkyl, C1-C6 alkyl ether), including isotopically enriched versions thereof. In some embodiments, this invention pertains to methods for the preparation of active esters of N-substituted piperazine acetic acid, including isotopically enriched versions thereof. For example, the isotopically labeled N-methylpiperazine II (R1 = 180H) reacted with the trifluoroacetic acid ester of N-hydroxysuccinimide to give the succinate II (R1 = OR2, R2 = succinimido). SSION NUMBER: 2005:592129 HCAPLUS

ACCESSION NUMBER:

DOCUMENT NUMBER:

143:97398

TITLE:

Preparation of active esters of N-substituted piperazine acetic acids, including isotopically

enriched versions

INVENTOR (S):

Dey, Subhakar; Pappin, Darryl J. C.; Purkayastha,

Subhasish; Pillai, Sasi; Coull, James M.

PATENT ASSIGNEE(S):

SOURCE:

Applera Corp., USA

U.S. Pat. Appl. Publ., 33 pp.

CODEN: USXXCO

DOCUMENT TYPE:

LANGUAGE:

Patent English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PAT	CENT :	NO.			KINI		DATE		1	APPL:	ICAT:	ION 1	10.		D	ATE	
	2005		71		A 1	;											
WO	2005				A1		2005						3		_	0050	
	W:	ΑE,	AG,	АL,	AM,	AT,	ΑU,	ΑZ,	BA,	BB,	BG,	BR,	BW,	BY,	BZ,	CA,	CH,
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		GE.	GH,	GM.	HR,	HU.	ID,	IL,	IN,	IS,	JP,	ΚE,	KG,	KΡ,	KR,	KZ,	LC,
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							PL,										
							TZ,										
	DM.		•	•	•		MW,	•									
	RW:																
							RU,										
		•	•	•			GR,				-	-					
		RO,	SE,	SI,	SK,	TR,	BF,	ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,
		MR,	NE,	SN,	TD,	TG											
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									1	US 2	004 -	7513	87		A 2	0040	105
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IT 856187-87-6P 856188-16-4P 856188-20-0P

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)

(preparation of active esters of N-substituted piperazine acetic acids and their labeled derivs.)

RN 856187-87-6 HCAPLUS

CN 2,5-Pyrrolidinedione, 1-[[(4-methyl-1-piperazinyl)acetyl-180]oxy]- (9CI) (CA INDEX NAME)

RN 856188-16-4 HCAPLUS

CN 2,5-Pyrrolidinedione, 1-[[(4-methyl-1-piperazinyl)acetyl-13C2-180]oxy]-, dihydrochloride (9CI) (CA INDEX NAME)

●2 HCl

RN 856188-20-0 HCAPLUS

CN 2,5-Pyrrolidinedione, 1-[[(4-methyl-1-piperazinyl-1-15N)acetyl-2-13C-180]oxy]-, dihydrochloride (9CI) (CA INDEX NAME)

●2 HCl

ANSWER 3 OF 7 HCAPLUS COPYRIGHT 2005 ACS on STN L6 ED Entered STN: 08 Jul 2005 This invention pertains to mixts. of isobarically labeled analytes and fragment ions thereof. 2005:592027 HCAPLUS ACCESSION NUMBER: 143:93642 DOCUMENT NUMBER: Mixtures of isobarically labeled analytes and TITLE: fragments ions derived therefrom Pappin, Darryl J. C.; Purkayastha, Subhasish; Coull, INVENTOR(S): James M. Applera Corp., USA PATENT ASSIGNEE(S): U.S. Pat. Appl. Publ., 36 pp., Cont.-in-part of U.S. SOURCE: Ser. No. 751,353. CODEN: USXXCO DOCUMENT TYPE: Patent English LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION: APPLICATION NO. DATE PATENT NO. KIND DATE ______ _ _ _ _ _ _ _ _ _ _ _ 20050707 US 2004-822639 20040412 A1 US 2005147985 A1 20050707 US 2004-751353 20040105 US 2005147982 US 2005148087 US 2004-852730 20040524 A1 20050707 20050105 20050728 WO 2005-US223 WO 2005068446 A1 W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG US 2004-751353 A2 20040105 PRIORITY APPLN. INFO.: US 2004-751354 A 20040105 20040105 US 2004-751387 Α US 2004-751388 20040105 Α US 2004-822639 A2 20040412 A 20040524 US 2004-852730 856187-87-6P 856188-16-4P 856188-20-0P IT RL: SPN (Synthetic preparation); PREP (Preparation) (mixts. of isobarically labeled analytes and fragments ions derived

therefrom)

856187-87-6 HCAPLUS RN

2,5-Pyrrolidinedione, 1-[[(4-methyl-1-piperazinyl)acetyl-180]oxy]- (9CI) CN (CA INDEX NAME)

RN856188-16-4 HCAPLUS

2,5-Pyrrolidinedione, 1-[[(4-methyl-1-piperazinyl)acetyl-13C2-180]oxy]-, CN

dihydrochloride (9CI) (CA INDEX NAME)

•2 HCl

RN 856188-20-0 HCAPLUS
CN 2,5-Pyrrolidinedione, 1-[[(4-methyl-1-piperazinyl-1-15N)acetyl-2-13C180]oxy]-, dihydrochloride (9CI) (CA INDEX NAME)

•2 HCl

L6 ANSWER 4 OF 7 HCAPLUS COPYRIGHT 2005 ACS on STN

ED Entered STN: 08 Jul 2005

GI

Isotopically enriched N-substituted piperazine-1-acetic acids (I) or salts thereof, comprising one or more heavy atom isotopes [X = 0, S; Y =straight chain or branched C1-6 alkyl or C1-6 alkyl ether group wherein the carbon atoms of the alkyl group or alkyl ether group each independently comprise linked hydrogen, deuterium or F atoms; Z = independently H, deuterium, F, Cl, Br, iodine, an amino acid side chain, a straight chain or branched C1-6 alkyl group that may optionally contain a substituted or unsubstituted aryl group (wherein the carbon atoms of the alkyl and aryl groups each independently comprise linked H, deuterium or F atoms), a straight chain or branched C1-6 alkyl ether group that may optionally contain a substituted or unsubstituted aryl group wherein the carbon atoms of the alkyl and aryl groups each independently comprise linked H, deuterium or F atoms, or a straight chain or branched C1-6 alkoxy group that may optionally contain a substituted or unsubstituted aryl group (wherein the carbon atoms of the alkyl and aryl groups each independently comprise linked H, deuterium or F atoms)] are prepared N-substituted piperazines can be used as intermediates in the synthesis of N-substituted piperazine acetic acids which in turn can be used as intermediates in the synthesis of active esters of N-substituted piperazine acetic acid. The active esters of N-substituted piperazine acetic acid can be used as labeling reagents to prepare a set of isobaric labeling reagents. The set of isobaric labeling reagents can be used to label analytes such as peptides, proteins, amino acids, oligonucleotides, DNA, RNA, lipids, carbohydrates, steroids, small mols. and the like. Thus, to a stirring solution of 1.18 g (11.83 mmol) N-methylpiperazine in 15 mL toluene at room temperature was added 1 g (5.91 mmol) of Et bromoacetate-1,2-13C dropwise, over a period of 15 min. The reaction mixture was then heated in an oil bath at 90° for 4 h, cooled to room temperature, filtered to remove the off-white solid to give, after workup on the combined filtrate and washings, 1.10 g (quant.) of 4-methylpiperazine-1acetic acid Et ester-1,2-13C (II) as an off-white oil. II (1.1 g) was refluxed in water for 24 h to give 780 mg 4-methylpiperazine-1-acetic acid-1,2-13C.

ACCESSION NUMBER: 2005:588426 HCAPLUS

DOCUMENT NUMBER: 143:115568

TITLE: Preparation of isotopically enriched N-substituted

piperazine-1-acetic acids

INVENTOR(S):
Dey, Subhakar; Pappin, Darryl J. c.; Purkayastha,

Subhasish; Pillai, Sasi; Coull, James M.

PATENT ASSIGNEE(S): Applera Corp., USA

SOURCE: U.S. Pat. Appl. Publ., 29 pp.

CODEN: USXXCO

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 6

PATENT INFORMATION:

		APPLICATION NO.	
		US 2004-751387	20040105
W: AE, AG, AI CN, CO, CI GE, GH, GI LK, LR, LS NO, NZ, OI TJ, TM, TI RW: BW, GH, GI	AM, AT, AU, AZ, R, CU, CZ, DE, DK, M, HR, HU, ID, IL, S, LT, LU, LV, MA, M, PG, PH, PL, PT, TR, TT, TZ, UA, M, KE, LS, MW, MZ,	WO 2005-US223 BA, BB, BG, BR, BW, DM, DZ, EC, EE, EG, IN, IS, JP, KE, KG, MD, MG, MK, MN, MW, RO, RU, SC, SD, SE, UG, US, UZ, VC, VN, NA, SD, SL, SZ, TZ,	BY, BZ, CA, CH, ES, FI, GB, GD, KP, KR, KZ, LC, MX, MZ, NA, NI, SG, SK, SL, SY, YU, ZA, ZM, ZW UG, ZM, ZW, AM,
EE, ES, F	I, FR, GB, GR, HU, I, SK, TR, BF, BJ,	TM, AT, BE, BG, CH, IE, IS, IT, LT, LU, CF, CG, CI, CM, GA, US 2004-751353 US 2004-751384 US 2004-751387 US 2004-751388 US 2004-822639	MC, NL, PL, PT, GN, GQ, GW, ML, A 20040105 A 20040105 A 20040105 A 20040105
IT 856188-20-0P		US 2004-852730	

RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)

(preparation of isotopically enriched N-substituted piperazine-1-acetic acids as isobaric labeling reagents) 856188-20-0 HCAPLUS

RN

2,5-Pyrrolidinedione, 1-[[(4-methyl-1-piperazinyl-1-15N)acetyl-2-13C-CN 180]oxy]-, dihydrochloride (9CI) (CA INDEX NAME)

●2 HCl

IT 856188-16-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of isotopically enriched N-substituted piperazine-1-acetic acids as isobaric labeling reagents)

RN 856188-16-4 HCAPLUS

2,5-Pyrrolidinedione, 1-[[(4-methyl-1-piperazinyl)acetyl-13C2-180]oxy]-, CN dihydrochloride (9CI) (CA INDEX NAME)

●2 HCl

IT 856187-87-6P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of isotopically enriched N-substituted piperazine-1-acetic acids as isobaric labeling reagents)

RN 856187-87-6 HCAPLUS

CN 2,5-Pyrrolidinedione, 1-[[(4-methyl-1-piperazinyl)acetyl-180]oxy]- (9CI) (CA INDEX NAME)

L6 . ANSWER 5 OF 7 HCAPLUS COPYRIGHT 2005 ACS on STN

ED Entered STN: 08 Jul 2005

AB This invention pertains to isobarically labeled analytes and fragment ions

thereof.

ACCESSION NUMBER: 2005:588349 HCAPLUS

DOCUMENT NUMBER: 143:112150

TITLE: Isobarically labeled analytes and fragment ions

derived therefrom

INVENTOR(S): Pappin, Darryl J. C.; Purkayastha, Subhasish; Coull,

James M.

PATENT ASSIGNEE(S): Applera Corporation, USA

SOURCE: U.S. Pat. Appl. Publ.,

U.S. Pat. Appl. Publ., 88 pp., Cont.-in-part of U.S. Ser. No. 822,639.

CODEN: USXXCO

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.		APPLICATION NO.	DATE
US 2005148087	A1 20050707	US 2004-852730	20040524
US 2005147982	A1 20050707	US 2004-751353	20040105
US 2005147985	A1 20050707	US 2004-822639	20040412
WO 2005068446	A1 20050728	WO 2005-US223	20050105
W: AE, AG, AL,	AM, AT, AU, AZ,	BA, BB, BG, BR, BW,	BY, BZ, CA, CH,
CN, CO, CR,	CU, CZ, DE, DK,	DM, DZ, EC, EE, EG,	ES, FI, GB, GD,
GE, GH, GM,	HR, HU, ID, IL,	IN, IS, JP, KE, KG,	KP, KR, KZ, LC,
LK, LR, LS,	LT, LU, LV, MA,	MD, MG, MK, MN, MW,	MX, MZ, NA, NI,
		RO, RU, SC, SD, SE,	
TJ, TM, TN,	TR, TT, TZ, UA,	UG, US, UZ, VC, VN,	YU, ZA, ZM, ZW
		NA, SD, SL, SZ, TZ,	
		TM, AT, BE, BG, CH,	
		IE, IS, IT, LT, LU,	
RO, SE, SI,	SK, TR, BF, BJ,	CF, CG, CI, CM, GA,	GN, GQ, GW, ML,
MR, NE, SN,	TD, TG		
PRIORITY APPLN. INFO.:		US 2004-751353	A2 20040105
		US 2004-822639	A2 20040412
		US 2004-751354	
		US 2004-751387	
		US 2004-751388	
		US 2004-852730	A 20040524

IT 856187-87-6P

RL: SPN (Synthetic preparation); PREP (Preparation)

(isobarically labeled analytes and fragment ions derived therefrom)

RN 856187-87-6 HCAPLUS

CN 2,5-Pyrrolidinedione, 1-[[(4-methyl-1-piperazinyl)acetyl-180]oxy]- (9CI) (CA INDEX NAME)

L6 ANSWER 6 OF 7 HCAPLUS COPYRIGHT 2005 ACS on STN

ED Entered STN: 08 Jul 2005

AB This invention pertains to mixts. of isobarically labeled analytes and

fragment ions thereof.

ACCESSION NUMBER: 2005:588336 HCAPLUS

DOCUMENT NUMBER:

143:93635

TITLE:

Mixtures of isobarically labeled analytes and

fragments ions derived therefrom

INVENTOR (S):

Pappin, Darryl J. C.; Purkayastha, Subhasish; Coull,

James M.

PATENT ASSIGNEE(S):

Applera Corporation, USA

SOURCE:

U.S. Pat. Appl. Publ., 29 pp.

CODEN: USXXCO

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT: 6

PATENT INFORMATION:

PATENT NO.	KIND	DATE		
US 2005147982 US 2005147985 US 2005148087 WO 2005068446 W: AE, AG, CN, CO, GE, GH, LK, LR, NO, NZ, TJ, TM, RW: BW, GH, AZ, BY, EE, ES, RO, SE,	A1 A1 A1 A1 A1 A1 A1 AL, AM, AT CR, CU, CZ GM, HR, HU LS, LT, LU OM, PG, PH TN, TR, TT GM, KE, LS KG, KZ, ME FI, FR, GE SI, SK, TR SN, TD, TO	20050707 20050707 20050707 20050728 T, AU, AZ, Z, DE, DK, J, ID, IL, J, LV, MA, H, PL, PT, T, TZ, UA, S, MW, MZ, O, RU, TJ, G, GR, HU, R, BF, BJ,	US 2004-751353 US 2004-822639 US 2004-852730 WO 2005-US223 BA, BB, BG, BR, BW, DM, DZ, EC, EE, EG, IN, IS, JP, KE, KG, MD, MG, MK, MN, MW, RO, RU, SC, SD, SE, UG, US, UZ, VC, VN, NA, SD, SL, SZ, TZ, TM, AT, BE, BG, CH, IE, IS, IT, LT, LU, CF, CG, CI, CM, GA, US 2004-751353 US 2004-751354	20040105 20040412 20040524 20050105 BY, BZ, CA, CH, ES, FI, GB, GD, KP, KR, KZ, LC, MX, MZ, NA, NI, SG, SK, SL, SY, YU, ZA, ZM, ZW UG, ZM, ZW, AM, CY, CZ, DE, DK, MC, NL, PL, PT, GN, GQ, GW, ML,
			US 2004-751354 US 2004-751387 US 2004-751388 US 2004-822639 US 2004-852730	A 20040105 A 20040105 A2 20040412

IT 856187-87-6P

RL: SPN (Synthetic preparation); PREP (Preparation)

(mixts. of isobarically labeled analytes and fragments ions derived therefrom)

RN 856187-87-6 HCAPLUS

CN 2,5-Pyrrolidinedione, 1-[[(4-methyl-1-piperazinyl)acetyl-180]oxy]- (9CI) (CA INDEX NAME)

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ANSWER 7 OF 7 HCAPLUS COPYRIGHT 2005 ACS on STN
L6
     Entered STN: 20 Aug 2004
ED
AB
     This invention pertains to methods, mixts., kits and/or compns. for the
     determination of analytes by mass anal. using unique labeling reagents or sets of
     unique labeling reagents. The labeling reagents can be isomeric or
     isobaric and can be used to produce mixts. suitable for multiplex anal. of
     the labeled analytes.
ACCESSION NUMBER:
                          2004:681717 HCAPLUS
DOCUMENT NUMBER:
                          141:202794
                          Methods, mixtures, kits and compositions pertaining to
TITLE:
                          analyte determination
                          Pappin, Darryl J. C.; Bartlet-Jones, Michael
INVENTOR(S):
                          Applera Corporation, USA
PATENT ASSIGNEE(S):
                          PCT Int. Appl., 105 pp.
SOURCE:
                          CODEN: PIXXD2
DOCUMENT TYPE:
                          Patent
LANGUAGE:
                          English
FAMILY ACC. NUM. COUNT:
PATENT INFORMATION:
                                              APPLICATION NO.
                                                                      DATE
                          KIND
                                 DATE
     PATENT NO.
                          ----
     WO 2004070352
                          A2
                                 20040819
                                             WO 2004-US2077
                                                                      20040127
         W: AE, AE, AG, AL, AL, AM, AM, AM, AT, AT, AU, AZ, AZ, BA, BB, BG,
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             ES, FI, FI, GB, GD, GE, GE, GH, GM, HR, HR, HU, HU, ID, IL, IN,
             IS, JP, JP, KE, KE, KG, KG, KP, KP, KP, KR, KR, KZ, KZ, KZ, LC,
             LK, LR, LS, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MX,
             MZ, MZ, NA, NI
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             MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN,
             GQ, GW, ML, MR, NE, SN, TD, TG, BF, BJ, CF, CG, CI, CM, GA, GN,
             GQ, GW, ML, MR, NE, SN, TD, TG
                                              CA 2004-2488584
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                           AΑ
                                 20040819
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     US 2004219685
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     US 2004220412
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     US 2004219686
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                                              US 2003-443612P
                                                                      20030130
PRIORITY APPLN. INFO.:
                                              WO 2004-US2077
                                                                   W
                                                                     20040127
     741683-77-2P 741683-78-3P 741683-86-3P
     741683-93-2P
     RL: SPN (Synthetic preparation); PREP (Preparation)
         (methods, mixts., kits and compns. pertaining to analyte determination)
     741683-77-2 HCAPLUS
RN
     2,5-Pyrrolidinedione, 1-[(4-morpholinylacetyl-1-13C)oxy]- (9CI)
CN
     NAME)
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RN 741683-78-3 HCAPLUS 2,5-Pyrrolidinedione, 1-[(4-morpholinylacetyl-2-13C)oxy]- (9CI) CN NAME)

RN 741683-86-3 HCAPLUS

CN 2,5-Pyrrolidinedione, 1-[(1-piperidinylacetyl-1-13C)oxy]- (9CI) (CA INDEX NAME)

RN 741683-93-2 HCAPLUS

CN 2,5-Pyrrolidinedione, 1-[(1-piperidinylacetyl-2-13C)oxy]- (9CI) (CA INDEX NAME)

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FULL ESTIMATED COST	37.03	202.01
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-5.11	-5.11

STN INTERNATIONAL LOGOFF AT 15:51:21 ON 08 SEP 2005